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Model Hamiltonians of open quantum optical systems: Evolvement from hermiticity to adjoint commutativity

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Abstract. In the conventional quantum mechanics of conserved systems, Hamiltonian is assumed to be a Hermitian operator. However, when it comes to quantum systems in presence of dissipation and/or noise, including open quantum optical systems, the strict hermiticity requirement is nor longer necessary. In fact, it can be substantially relaxed: the non-Hermitian part of a Hamiltonian is allowed, in order to account for effects of dissipative environment, whereas its Hermitian part would be describing subsystem's energy. Within the framework of the standard approach to dissipative phenomena based on a master equation for the reduced density operator, we propose a replacement of the hermiticity condition by a more general condition of commutativity between Hermitian and anti-Hermitian parts of a Hamiltonian. As an example, we consider a dissipative two-mode quantum system coupled to a single-mode electromagnetic wave, where we demonstrate that the adjoint-commutativity condition does simplify the parametric space of the model.

1. Introduction

In a conventional quantum mechanics of conserved systems, Hamiltonian is assumed to be a Hermitian operator operating in a suitably chosen Hilbert space. This hermiticity ensures real-valued energy eigenvalues and seems to be sufficient when dealing with conserved systems.

But what if our Hamiltonian has a non-Hermitian part (also known as anti-Hermitian or skew-adjoint, depending on a context)? At first glance, this generalization might bring imaginary parts into energy (eigen)values, which would be in an obvious contradiction with energy's physical meaning. It turns out however that non-Hermitian parts do not act that way in Hamiltonians, if they are being properly implemented. Instead of inducing complex energy values, non-Hermitian parts can describe changes of energy, which could occur, for instance, due to the effect of dissipative environment, as we shall discuss in the next section.

The first attempts to apply non-Hermitian Hamiltonians to open quantum and quantum-optical systems can be traced as far back as 1950s, or even before [1, 2, 3]. A modern version of the density operator approach with non-Hermitian Hamiltonians has been proposed relatively recently [4, 5, 6], where the normalization transformation was introduced. This immediately resulted in an outburst of applications, including entanglement's generation, amplification and protection, decoherence, spin squeezing, dissipative dimers, spin-chain-star systems, kicked rotor models, violations of Leggett–Garg inequality, population dynamics, Bayesian parameter estimation, modifications of the two-point measurement method, macroscopic quantum electrodynamics with a pseudomode, coherence delocalization in coupled-cavity systems, models with non-local initial conditions, nuclear spin ensemble with a reservoir, adiabaticity and entropy dynamics of various two-level dissipative systems, quantum Fisher information and phase estimation without and with decoherence, ground-state cooling of near-degenerate mechanical modes, to mention only a recent literature [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28].

The main idea of the approach is the following. Suppose we have a quantum-mechanical system, which is initially conservative and isolated from any environment; all its properties are encoded in a density operator. For a conservative system, its density operator's evolution is governed by the von Neumann equation, which is the quantum mechanical analogue of the classical Liouville equation. Now, at some moment of time, we "switch" environment on. Then our system becomes a subsystem, its density operator must be treated as a *reduced density* operator [3]. This density operator's evolution is now governed by a generalization of the von Neumann equation called the *master equation.* The latter must take into account the effect of the environment, which can affect both the (sub)system's Hamiltonian and the Liouvillian part of its evolution (master) equation.

There are different approaches to how to quantify this effect of the environment while studying the subsystem alone. For example, Lindblad approach uses a large set of approximations, including the Markovian process, to derive the correction to the Liouvillian part of the evolution equation; this correction turns out to be of a semi-group form. On the contrary, the non-Hermitian Hamiltonian approach does not use the above-mentioned approximations. Instead, it is rooted in the fact that environment can shift the poles of the system's scattering amplitudes or propagators or other observable parameters, which can be formally accounted for by adding anti-Hermitian corrections to the Hamiltonian. According to the approach [4, 5, 6], those corrections must be viewed not as a part of the Hamiltonian but as a contribution to the Liouvillian part of an evolution equation for reduced density operator.

2. Master equation

In this section, we present the master equation, which is a natural generalization of the conventional quantum-mechanical Liouville-von Neumann equation for the case of dissipative quantum and semiclassical systems.

To begin with, in our approach, it will be assumed that the dissipative effects are encoded in anti-Hermitian terms of the subsystem's Hamiltonian, as discussed in the Introduction. In other words, in this approach one deals exclusively with the degrees of freedom of the subsystem, whereas all degrees of freedom of environment have been averaged ("integrated out").

Thus, our (sub)system non-Hermitian Hamiltonian operator is partitioned into Hermitian and anti-Hermitian parts

$$\hat{H} = \hat{H}_+ + \hat{H}_-, \tag{1}$$

where we denoted $\hat{H}_\pm = \pm\hat{H}_\pm^\dagger = \frac{1}{2}(\hat{H} \pm \hat{H}^\dagger)$. It is sometimes convenient to introduce a self-adjoint operator $\hat{\Gamma} \equiv i\hat{H}_-$ which will be referred as the *decay rate operator* throughout the paper.

The next step is to introduce the normalized density operator, $\hat{\rho}' = \hat{\rho}'(t)$, as a primary physical statistical object of the theory. Compared to a state vector, the main advantage of the density operator is that it is capable of handling not only pure states but also mixed states. This is an important feature when dealing with open systems, because pure states can evolve into mixed states with time, see [6] and references therein, hence one needs to employ an approach with maximum generality possible.

According to quantum statistical mechanics, an average of a quantum observable $\hat{O}$ is defined as $\langle O\rangle_{\rm obs} \equiv {\rm tr}\left(\hat{\rho}'\hat{O}(0)\right)$.

Let us determine the evolution equation for the density operator. In ref. [5], the following equation was proposed

$$\begin{aligned} \frac{d}{dt}\hat{\rho}'(t) &= -\frac{i}{\hbar}\left(\hat{H}\hat{\rho}'(t) - \hat{\rho}'(t)\,\hat{H}^\dagger\right) + \frac{2i}{\hbar}{\rm tr}\left(\hat{\rho}'(t)\hat{H}_-\right)\hat{\rho}'(t) + \hat{D}(\rho'(t), A_k) \\ &= -\frac{i}{\hbar}\left[\hat{H}_+, \hat{\rho}'(t)\right] - \frac{i}{\hbar}\left\{\hat{H}_-, \hat{\rho}'(t)\right\} + \frac{2i}{\hbar}{\rm tr}\left(\hat{\rho}'(t)\hat{H}_-\right)\hat{\rho}'(t) + \hat{D}(\rho'(t), A_k), \end{aligned} \tag{2}$$

where $\hat{D}(\rho, A_k)$ is dubbed as the dissipator - a traceless, linear operator in terms of the density operator, quadratic in terms of the Lindblad operators $\hat{A}_k$, $k = 1, ..., N^2 - 1$ and $N = \dim(\mathcal{H}_S)$, Using quantum dynamical semigroup formalism, the dissipator can be shown to have the form [3]:

$$\hat{D}(\rho, A_k) = \sum_{k=1}^{N^2-1} \gamma_k \left(\hat{A}_k\hat{\rho}\hat{A}_k^\dagger - \frac{1}{2}\hat{A}_k^\dagger\hat{A}_k\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{A}_k^\dagger\hat{A}_k\right), \tag{3}$$

where γ's are non-negative quantities which can be derived from correlation functions of the environment; they usually play the role of relaxation rates for different decay modes. The dissipator describes, together with the non-Hermitian Hamiltonian part, the dissipative effects of the environment.

Essentially, by this equation we unify the Lindblad master equation approach with the non-Hermitian Hamiltonian formalism for the density matrix. Note that dissipator and non-Hermitian Hamiltonian parts have a different physical nature and origins and thus should describe different types of dissipation, as discussed in the Introduction. Therefore, resulting "hybrid" equation (2) is expected to have a larger applicability range than any of these two approaches taken separately, because the Lindblad and non-Hermitian Hamiltonian parts have different physical origins.

For practical purposes of finding solutions of the master equation, it is convenient to search for normalized density operator using a following ansatz:

$$\hat{\rho}'(t) = \hat{\rho}(t)/{\rm tr}\left(\hat{\rho}(t)\right), \tag{4}$$

and write down evolution equations in terms of $\hat{\rho}(t)$ alone. From (2) we obtain the following equations for $\hat{\rho}(t)$

$$\begin{aligned} \frac{d}{dt}\hat{\rho}(t) &= -\frac{i}{\hbar}\left(\hat{H}\hat{\rho}(t) - \hat{\rho}(t)\,\hat{H}^\dagger\right) + \hat{D}(\rho(t), A_k) \\ &= -\frac{i}{\hbar}\left[\hat{H}_+, \hat{\rho}(t)\right] - \frac{i}{\hbar}\left\{\hat{H}_-, \hat{\rho}(t)\right\} + \hat{D}(\rho(t), A_k). \end{aligned} \tag{5}$$

One can see that equations for $\hat{\rho}$ are not only shorter but also nor longer contain terms nonlinear with respect to $\hat{\rho}$. This can significantly facilitate their solving, in either analytical or numerical workflow.

3. Adjoint commutativity

Ideally, a full Hamiltonian (both its Hermitian and anti-Hermitian parts) of an open quantum system must be derived from an underlying microscopic physics of a subsystem and its environment. However, the underlying physics of a subsystem often involves many-body systems of quantum particles, whereas an environment has not only the many-body system's complexity but also a large degree of diversity and uncertainty. All this requires tremendous computational power and/or causes enormous analytical difficulties.

Therefore, it is important to establish as many universal features of Hamiltonians as possible. In some cases, this can provide more clear understanding of underlying physical processes and phenomena. Since we cannot use the hermiticity requirement anymore, as mentioned in the introductory section, its generalizations must be considered instead of.

One possible way would be to replace the hermiticity of a full Hamiltonian with commutativity of its Hermitian and anti-Hermitian parts:

$$[\hat{H}, \hat{H}^{\dagger}] = 0 \quad \Leftrightarrow \quad [\hat{H}_{+}, \hat{H}_{-}] = 0, \tag{6}$$

which is equivalent to the commutativity condition between the following two Hermitian operators:

$$[\hat{H}_{+}, \hat{\Gamma}] = 0, \tag{7}$$

if we recall notations made after equation (1).

The importance of the condition (7) is it implies that we can measure observables related to the $\hat{H}_{+}$ and decay rate operators simultaneously with arbitrarily good precision. In other words, $\hat{H}_{+}$ and $\hat{\Gamma}$ are compatible observables, hence they admit a common set of eigenvectors, *i.e.*, there exists a complete basis of eigenvectors $|\psi_n\rangle$ which simultaneously satisfies relations

$$\hat{H}_{+}|\psi_n\rangle = E_n|\psi_n\rangle, \ \hat{\Gamma}|\psi_n\rangle = \Gamma_n|\psi_n\rangle, \tag{8}$$

where values E and Γ usually have a physical meaning of the subsystem's energy and decay rate, respectively. Thus, E and Γ are quantum numbers which can be observed simultaneously with arbitrarily good precision, according to the generalized Heisenberg principle

$$\mathrm{Var}(E)\,\mathrm{Var}(\Gamma) \geq \frac{1}{4}\left|\langle[\hat{H}_{+}, \hat{\Gamma}]\rangle\right|^2 = 0, \tag{9}$$

where $\mathrm{Var}(X) \equiv \langle X^2\rangle - \langle X\rangle^2$ is variance of a physical variable described by the operator $\hat{X}$.

In terms of consecutive measurements, if condition (7) holds, then the order of measurements of E and Γ does not affect the probabilities, as they are both calculated with the same eigenstate $|\psi_n\rangle$. After two measurements, the state of system is a joint eigenstate, in which observables E and Γ are both well defined. If condition (7) does not hold, the order of measurements matters, because the state of the system after, say, two experiments is an eigenfunction of a last measured observable. In this state, only the second, but not the first, observable is well defined, therefore, for instance, a third measurement, which measures again the first observable, would return a different value from the first measurement.

4. Example: two-level quantum optical system

In quantum optics, two-level systems (TLS) find many applications, due to their physical clarity and mathematical simplicity. It is thus natural to consider it as an example for the purposes of our study. This is primarily due to the fact that the two-level approach occurs as a robust or leading approximation for many quantum systems, such as those in which energy differences between two groups of levels are much larger than levels' splittings themselves.

Let us thus consider a two-level atom (a dipole), which can "decay" from excited to ground state by the emission of a photon. This can occur due to the interaction of the atom with the surrounding background, or vacuum in this case. The complete quantum system would be 'atom plus photons plus vacuum' one in this case, but we are interested only in time dependence of the atom's state.

Therefore, a (sub)system we consider here is defined by the Hamiltonian

$$\hat{H}_+^{(a)} \equiv \hat{H}_0 + \hat{H}_L,\ \hat{H}_0 = \frac{1}{2}\hbar\omega_0\hat{\sigma}_3,\ \hat{H}_L = \frac{1}{2}\hbar\Omega\hat{h}_{+-}, \tag{10}$$

where we denoted $\hat{h}_{+-} = \mathrm{e}^{-i\omega_0 t}\hat{\sigma}_+ + \mathrm{e}^{i\omega_0 t}\hat{\sigma}_-$ and $\hat{\sigma}_\pm = \frac{1}{2}\left(\hat{\sigma}_1 \pm i\hat{\sigma}_2\right)$, σ's being the Pauli matrices. It is an explicitly Hermitian operator on a two-dimensional Hilbert space. The unperturbed part of Hamiltonian, $\hat{H}_0$, represents energy levels of a free dipole, while the perturbation term $\hat{H}_L$ describes the interaction between the dipole and electromagnetic wave (a single mode).

An anti-Hermitian part to be added to $\hat{H}_+^{(a)}$, to form a complete Hamiltonian of our model, is

$$\hat{H}_-^{(a)} \equiv -i\hat{\Gamma}^{(a)} = \hat{H}_\lambda + \hat{H}_D + \hat{H}_{00},\ \hat{H}_\lambda = \frac{1}{2}i\hbar\lambda\hat{\sigma}_3,\ \hat{H}_D = -\frac{1}{2}i\hbar\alpha\hat{h}_{+-},\ \hat{H}_{00} = -\frac{1}{2}i\hbar\mathcal{T}\hat{I}, \tag{11}$$

where λ, α and $\mathcal{T}$ being real-valued free parameters.

The Hamiltonian $\hat{H}_\lambda \propto \hat{\sigma}_+\hat{\sigma}_-$ occurs in studies of photodetection and it is related to continuous measurements in presence of radiation modes [3]. Its anti-Hermitian counterpart would be the term $\hat{H}_D$, therefore, $\hat{H}_D$ is supposed to describe the dissipative processes during the dipole interaction between an atom and external electromagnetic wave field.

It is convenient to do computations in the interaction picture which can be achieved by performing a unitary transformation of the density operator, $\hat{\rho}(t)$ in this case, which results in the following mappings:

$$\begin{gathered}
\hat{\rho} \mapsto \hat{\rho}_{(I)},\ \left[\hat{H}_0, \hat{\rho}\right] \mapsto 0,\ \hat{H}_L \mapsto \frac{1}{2}\hbar\Omega\left(\hat{\sigma}_+ + \hat{\sigma}_-\right) = \frac{1}{2}\hbar\Omega\hat{\sigma}_1, \\
\vec{\sigma} \mapsto \begin{pmatrix} \cos(\omega_0 t) & \sin(\omega_0 t) & 0 \\ -\sin(\omega_0 t) & \cos(\omega_0 t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \vec{\sigma},\ \ \hat{\sigma}_\pm \mapsto \mathrm{e}^{\pm i\omega_0 t}\hat{\sigma}_\pm,
\end{gathered}$$

where a subscript (I) denotes the interaction-picture transform of a value.

Upon applying the above-mentioned transformations, the evolution equation of our model transforms into the interaction-picture form:

$$\begin{aligned}
\frac{d}{dt}\hat{\rho}_{(I)} = {} & \frac{i\Omega}{2}\left[\hat{\sigma}_+ + \hat{\sigma}_-, \hat{\rho}_{(I)}\right] - \frac{\alpha}{2}\left\{\hat{\sigma}_+ + \hat{\sigma}_-, \hat{\rho}_{(I)}\right\} + \gamma_1\left(\hat{\sigma}_-\hat{\rho}_{(I)}\hat{\sigma}_+ - \frac{1}{2}\{\hat{\sigma}_+\hat{\sigma}_-, \hat{\rho}_{(I)}\}\right) \\
& + \frac{\lambda}{2}\left\{\hat{\sigma}_3, \hat{\rho}_{(I)}\right\} - \mathcal{T}\hat{\rho}_{(I)},
\end{aligned} \tag{12}$$

where Pauli matrices $\hat{\sigma}_-$ and $\hat{\sigma}_+$ play the roles of the Lindblad operators $\hat{A}_1$ and $\hat{A}_1^\dagger$ in the interaction picture, respectively (in the definition (3), we assume that γ_k vanish for all $k > 1$).

One can see that behavior and solutions of these equations depends on five parameters of the model, ω_0, Ω, γ_1, α, λ (the gauge constant $\mathcal{T}$ can be chosen *ad hoc* for it does not occur in the normalized density operator). The values of the former three parameters can be established from underlying microscopic physics relatively easy. What can be done with determining the remaining two parameters, preferably without plunging into complexity of underlying multi-body dissipative processes?

Let us apply the formalism of section 3 in this regard. We thereby assume that the energy and decay rate of the system described by the total Hamiltonian (10), (11) are simultaneously observable physical values:

$$\hat{H}_+^{(a)}|\psi_n\rangle = E_n^{(a)}|\psi_n\rangle,\ \hat{\Gamma}^{(a)}|\psi_n\rangle = \Gamma_n^{(a)}|\psi_n\rangle, \tag{13}$$

according to equations (8). Applying the commutativity condition (7) to the non-Hermitian Hamiltonian (10), (11), we arrive at the following equation

$$[\hat{H}_{+}^{(a)}, \hat{\Gamma}^{(a)}] = \frac{\hbar^2}{4}(\alpha\,\omega_0 + \lambda\,\Omega)[\hat{h}_{+-},\, \hat{\sigma}_3] = 0, \tag{14}$$

which, if taken at arbitrary time, results in a constraint for the parameters of our model:

$$\frac{\alpha}{\lambda} = -\frac{\Omega}{\omega_0}. \tag{15}$$

This identity not only decreases a number of unknown parameters of the model by one, but also brings us, if empirically confirmed, some important information about how dissipative effects acting upon the dipole atom system depend on, and interplay with, the “conservative” characteristics thereof.

5. Conclusion

In the conventional quantum mechanics of conserved systems, Hamiltonian is assumed to be a Hermitian operator, in order to ensure real-valued eigenvalues of energy. However, when it comes to quantum systems in presence of dissipation and/or noise, including open quantum optical systems, the strict hermiticity requirement is nor longer necessary. In fact, it can be substantially relaxed: the non-Hermitian part of a Hamiltonian is allowed, in order to account for effects of dissipative environment, whereas its Hermitian part would be describing subsystem’s energy.

In this talk, within the framework of the standard approach to dissipative phenomena based on a master equation for the reduced density operator, we study a possible replacement of the hermiticity condition. Instead of hermiticity condition $\hat{H} = \hat{H}^\dagger$, we propose a more general condition based on commutation relations between Hermitian and anti-Hermitian parts of a Hamiltonian - the adjoint commutativity: $[\hat{H}, \hat{H}^\dagger] = 0$. The adjoint commutativity implies that we can measure simultaneously with arbitrarily good precision the observables described by the operators of subsystem’s energy $\hat{H}_+$ and decay rate $\hat{\Gamma}$.

As an example, we consider a dissipative two-mode quantum system coupled to a single-mode electromagnetic wave. We demonstrate how the adjoint commutativity condition yields at least one constraint upon parameters of the model.

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